Direct Numerical Tests of Kinetic Theory Collision Integrals with Molecular Dynamics Simulations of Stopping Power in Plasmas

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Molecular dynamics (MD) is used as a validation tool for different stopping models based on kinetic theory. MD is also used to improve those models so they are accurate over a wider range of conditions. Unlike many transport quantities, stopping is difficult to accurately model because one must reproduce a function of projectile velocity instead of an average over a velocity distribution. Our new models are accurate to within a few percent. These models can now be used to derive general transport coefficients.

All of transport theory (diffusion, thermal conductivity, electrical conductivity, stopping power, etc.) of non-zero mass particles is derived from kinetic theory, in which a phase space distribution function is evolved in time. Calculating the correct evolution is dependent on having the right collision operator that models how small-distance and small-time interactions between particles change, and eventually thermalize, the distribution. MD simulations provide an ideal numerical laboratory in which different classical kinetic theories can be tested and broken by directly simulating all inter-particle interactions, and hence the full many-body phase-space distribution.

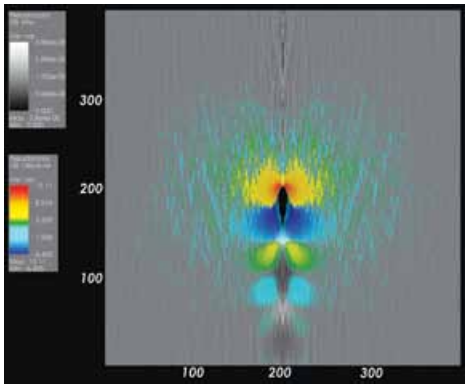

Fig. 1. The wake field is shown for a Z=-2 projectile near the center of the image, moving in the positive y direction. The field of view is 720 Å, compared to the cell length of 1075 Å; the screening length is 2.4 Å. The electron charge density, ρ, is shown in gray; the strongly-repulsive screening cloud is the dark lozenge. The logarithm of the energy transfer field, φ, is shown in color. (Specifically, Sign (φ) ln $|\varphi|$ is shown with a cutoff at small values.) The result is time-averaged over the 400 fs duration of the simulation and is cylindrically-averaged around the axis of the particle trajectory.

The mean energy loss of a projectile per unit distance *(dE/dx*), or stopping power, in a classical target was chosen as our observable of interest for three reasons: (1) it is the only velocity-resolved transport property, (2) the classical linear response theory leads to a divergent answer without an ad hoc cutoff at small distances, and (3) stopping power is itself an important property relevant to thermonuclear fusion in inertial confinement fusion devices, for both alpha particles produced during burn and for fast ignition heating of the target. Therefore, stopping power is both the most difficult transport quantity to model correctly and of major relevance to the core mission of LANL.

MD simulations were performed with the two-time Gordon Bell prize winning code ddcMD, originally developed at LLNL and now ported to the LANL supercomputer, Cielo. The code ddcMD is capable of simulating billions of particles with long-range forces and is a virtual plasma laboratory and workhorse code of the Cimarron project [1]. Recently, it has been used to study electron-ion temperature equilibration [2], fusion enhancement rates [3], and ignition [4] while thermal conductivity and interface diffusion results are in progress.

We have studied a wide range of conditions, varying the Coulomb coupling parameter of the target, $\Gamma_t = e^2/ak_BT$, a measure of the ratio of mean potential energy e^2/a, where a is the electron sphere radius, to mean kinetic energy k_BT in the system, from $\Gamma_t = 0.1$ (near pure hydrogen plasma at thermonuclear burn conditions) to *10.0* (stopping power experimental conditions), and using three different types of projectiles: (1) anti-protons ($Z = -1$), (2) anti-alpha particles ($Z = -2$), and (3) anti-Neon nuclei ($Z = -10$). Note that because the projectiles have the same charge as the electrons, we do not study the bound component of stopping.

Figure 1 shows the electron density, ρ, around a moving anti-alpha particle ($v \sim 9\, v_{th}$), and a color image of the energy deposition field, φ, is superimposed. This is the differential work performed on the target electrons by the projectile. Both fields are time and azimuthal averages of the instantaneous particle distributions. For this case, the major part of the energy transfer occurs in front of the projectile via strong particle-particle collisions with the electrons in the target. The dynamic collective response leads to damped plasma oscillations in the tail behind the moving projectile. These are visible in the grayscale density ρ and in the faint alternations in the energy flow from projectile to target. The wavelength in the wake scales as the product of the projectile velocity and plasma oscillation. In the future, we will generalize this to a two-component plasma in which separate current-density fields of electrons and fuel ions will be used to compute the electron-fuel energy split.

Figure 2 shows the unitless low velocity friction coefficient $R = \lim_{v\to 0}(dE/dx)\lambda^2 v_{th}/vZ^2e^2$, where λ is the Debye length, v_{th} is the thermal velocity, v is the velocity of the projectile and Ze is the projectile charge. This quantity is related to the diffusion coefficient [5], which can be obtained via a fit to molecular dynamics [6]. Another model valid at low velocities is the T-matrix model, which depends on a cross-section through the Boltzmann collision integral. The use of the Coulomb

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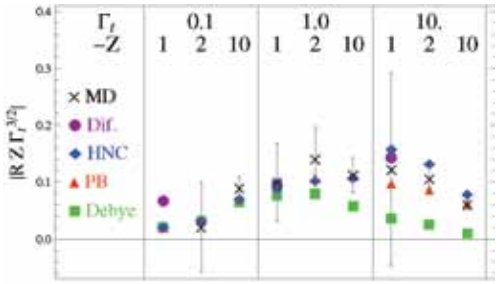

Fig. 2. The friction coefficient over a range of different Coulomb coupling parameters and projectile charges. Results are shown for MD (black crosses with error bars), the diffusion model of Dufty (purple circles), and T-matrix with a screening potentials derived from hypernetted chain (blue diamonds), the Poisson-Boltzmann equation (red triangles), and Debye-Huckel theory (green squares).

cross-section would be unphysical because real interactions are screened by the medium; furthermore, that result would be divergent. The screening cloud about the projectile can be calculated to high accuracy with the hypernetted chain approximation (HNC) [7]. Alternatively, one can solve the non-linear Poisson-Boltzmann (PB) equation, which assumes a Boltzmann distribution of electron energies and Coulomb interactions between particles. The linear version of this equation leads to simple Debye screening. Cross-sections from all three of these screening models are used and compared. We see that at small coupling, the choice of potential does not matter, but at large coupling the Debye potential will significantly underestimate the stopping.

The full stopping curve is a function of the velocity of the projectile. Static models break down when v is about v_{th} or greater, so a dynamic screening model is needed. Within linear response, one can write the random phase approximation (RPA) to the dielectric function and calculate the stopping, but this model breaks down at low velocities, where binary collisions make up the majority of the stopping. Gould and DeWitt [8] corrected for this behavior by adding in the T-matrix result and then subtracting the static RPA result in order to avoid double counting. This model works well at small coupling but breaks down at strong coupling. Zwicknagel [9] instead used the T-matrix method with the slight change of scaling the screening length with velocity to match the high-velocity Bohr limit. This works very well, but tends to underestimate the stopping by *10–15%* (and more at low velocities) for moderate to strong coupling. We have made two improvements to this model: (1) we use more accurate potentials in the T-matrix model, and (2) we have altered the scaling factor to better match the MD data at moderate to high velocities. Figure 3 compares these models at small and large coupling.

In summary, MD is a powerful tool for validating models that are used in hydrodynamics and kinetic theory codes. We have used it here to test stopping models over a wide range of conditions and to develop improved models able to match the MD data to within a couple of percent. These models are now validated at the velocity resolved level and can be used more generally in other transport calculations.

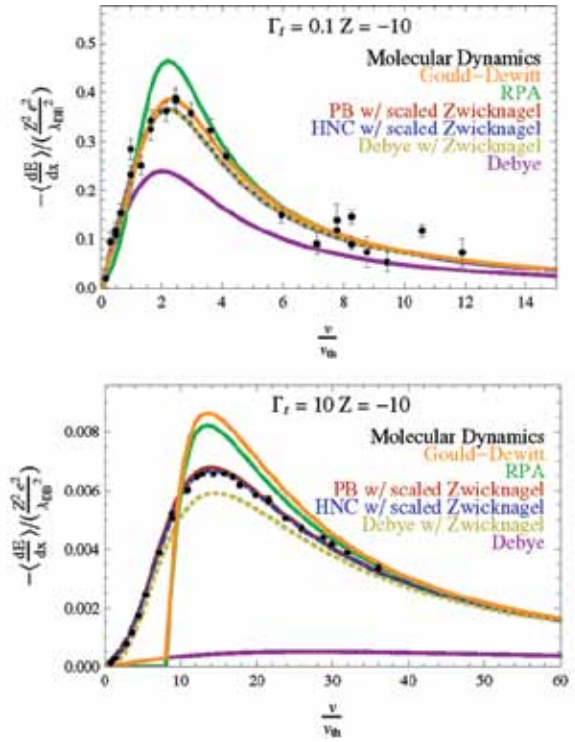

Fig. 3. The stopping power as a function of velocity for an anti-Neon projectile in a weakly and strongly coupled electron target. Results are shown for MD (black dots with error bars), the combined model of Gould and Dewitt (orange), the random phase approximation (green), and T-matrix with a scaled screening potential derived from the PB equation (red), hypernetted chain (blue), and Debye-Huckel theory (yellow), and the unscaled Debye-Huckel potential (purple).

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